Homogenization of membrane and pillar photonic crystals

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Abstract

We study wave propagation and diffraction in a bidimensional photonic crystal with finite height, in case where the wavelength is large with respect to the period of the structure. The device is made of materials with anisotropic permittivity and permeability tensors. We derive rigorously the homogenized system, using the concept of two-scale convergence. The effective permittivity and permeability tensors turn out to be that of a two-dimensional photonic crystal with infinite height.

Photonic crystals, i.e. dielectric or metallic artificial periodic structures, are generally thought of as strongly scattering devices, authorizing the existence of photonic band gaps. However, their actual electromagnetic behavior when the wevelength is large with respect to the period is also interesting, because it can produce strongly anisotropic behaviors, plasmon frequencies, or even left-handed materials [1, 2]. The study of the properties of these structures in this asymptotic regime comes under the theory of homogenization [3]. A lot of results are by now very well-known both for 2D and 3D structures. In this paper, we consider a photonic crystal made of a collection of parallel finite-size fibers embedded in a matrix. This covers the case of structures made out of a layer of bulk materials in which holes are made periodically (membrane photonic crystal) but also the case of structures made out of nanopillars (pillar photonic crystal [4, 5, 6, 7, 8, 9]), or more generally, structures composed of fibers with finite length embedded in a matrix. Our point is to derive the effective permittivity and permeability tensors of this structure when the ratio between the period of the structure and the wavelength of the incident field is very small. We show, using the two-scale convergence method, that the effective, or homogenized, permittivity and permeability tensors of these structures are the same as that of infinitely long fibers, for which we had already derived rigorous results [10]. For infinitely long fibers, explicit formulas can be derived in some cases [3, 11, 12, 13]. Let us note that our results hold for dispersive and lossy materials.

The set of fibers is contained in a domain $\Omega = \mathcal{O} \times [-L, L]$ of $\mathbb{R}^3$ (cf. fig.1). The space coordinates are denoted: $\mathbf{x} = (x_1, x_2, x_3)$ and we also denote $\mathbf{x}_\perp = (x_1, x_2)$. The period of the lattice is denoted by η (see fig. 2). We denote by Y the basic two-dimensional cell of the lattice. The obstacle in Y is denoted by P. We consider time harmonic fields, the time dependence is chosen to be $\exp(-i\omega t)$. For a given monochromatic incident field $(\mathbf{E}^i, \mathbf{H}^i)$, we denote by $(\mathbf{E}^\eta, \mathbf{H}^\eta)$ the total electromagnetic field. Our aim is to pass to the limit $\eta \to 0$ and determine the limit of the couple $(\mathbf{E}^\eta, \mathbf{H}^\eta)$. In our methodology, we get at the limit a true electromagnetic scattering problem, for a given wavelength λ and a bounded obstacle Ω characterized by some permittivity and permeability tensors. This situation is quite different from other homogenization techniques, making use of periodization conditions, in which the frequency tends to zero, thus not leading to a diffraction problem but rather to an electrostatic one [14]. Such an approach can sometimes give useful explicit formulas but generally leads to complicated formulations. Moreover, it does not handle the boundary effects which

in some cases may lead to some miscomprehensions [15]. The relative permittivity tensor $\varepsilon^\eta(\mathbf{x})$ and relative permeability tensor $\mu^\eta(\mathbf{x})$ are described by :

$$\begin{cases} \varepsilon^\eta(\mathbf{x}) = \varepsilon_0 & \text{for } \mathbf{x} \in \mathbb{R}^3 \backslash \Omega \\ \varepsilon^\eta(\mathbf{x}) = \varepsilon^0\left(\frac{\mathbf{x}_\perp}{\eta}, x_3\right) & \text{for } \mathbf{x}_\perp \in \Omega \end{cases}, \begin{cases} \mu^\eta(\mathbf{x}) = \mu_0 & \text{for } \mathbf{x} \in \mathbb{R}^3 \backslash \Omega \\ \mu^\eta(\mathbf{x}) = \mu^0\left(\frac{\mathbf{x}_\perp}{\eta}, x_3\right) & \text{for } \mathbf{x}_\perp \in \Omega \end{cases} \tag{1}$$

where $\mathbf{y} \to \varepsilon^0(\mathbf{y}) = \left(\varepsilon^0_{ij}(\mathbf{y})\right)$ and $\mathbf{y} \to \mu^0(\mathbf{y}) = \left(\mu^0_{ij}(\mathbf{y})\right)$ are Y-periodic 3×3 matrix functions. The domain Ω is periodically filled with contracted cells $\eta Y \times [-L, L]$ (see fig. 2).

The total electromagnetic field $(\mathbf{E}^\eta, \mathbf{H}^\eta)$ satisfies

$$\begin{cases} \text{curl } \mathbf{E}^\eta = i\omega\mu_0\mu^\eta\mathbf{H}^\eta \\ \text{curl } \mathbf{H}^\eta = -i\omega\varepsilon_0\varepsilon^\eta\mathbf{E}^\eta \end{cases} \tag{2}$$

and $(\mathbf{E}^\eta - \mathbf{E}^i, \mathbf{H}^\eta - \mathbf{H}^i)$ satisfies Silver-Müller radiation conditions.

In order to describe this problem, we will rely on a two-scale expansion of the fields. That way, the physical problem is described by two variables: a macroscopic one $\mathbf{x}$ and a microscopic one $\mathbf{y}$ representing the rapid variations of the material at the scale of one basic cell, measured by η, that is, at the scale of ηY. By noticing that there are no rapid variations in the vertical direction x_3, the microscopic variable is set to be: $\mathbf{y} = \mathbf{x}_\perp/\eta$. Differential operators with respect to variable $\mathbf{y}$ are denoted with a subscript y. The fields are periodic with respect to that microscopic variable (this corresponds to the neighborhood of the Γ point in the first Brillouin zone). The limit problem obtained by letting η tend to 0, will then depend on the macroscopic, physical, variable $\mathbf{x}$ but also on the microscopic, hidden, variable $\mathbf{y}$. The total limit fields will read $\mathbf{E}^0(x, y)$ and $\mathbf{H}^0(x, y)$ and the observable, physical, fields will be given by the mean value over the hidden variable $\mathbf{y}$: $\mathbf{E}(x) = |Y|^{-1}\int_Y \mathbf{E}^0(x, y)\,dy$ and $\mathbf{H}(x) = |Y|^{-1}\int_Y \mathbf{H}^0(x, y)\,dy$, where $|Y|$ is the measure area of Y. In order to lighten the notations, we denote by brackets the averaging over Y, hence $\mathbf{H}(x) = \langle\mathbf{H}^0\rangle$ and $\mathbf{E}(x) = \langle\mathbf{E}^0\rangle$.

The main mathematical tool that we use is a mathematically clean version of the multiscale expansion, widely used in various areas of physics. More precisely, for a vector field $\mathbf{F}^\eta$ in $\left(L^2(\Omega)\right)^3$, we say, by definition, that $\mathbf{F}^\eta$ two-scale converges towards $\mathbf{F}^0$ if for every sufficiently regular function $\phi(\mathbf{x}, \mathbf{y})$, Y-periodic with respect to $\mathbf{y}$, we have:

$$\int_\Omega \mathbf{E}^\eta(\mathbf{x}) . \phi(\mathbf{x}, \mathbf{x}_\perp/\varepsilon)\,dx \to \iint_{\Omega\times Y} \mathbf{E}^0(\mathbf{x}, \mathbf{y}) . \phi(\mathbf{x}, \mathbf{y})\,dxdy, \tag{3}$$

as η tends to 0.

The limit field $\mathbf{F}^0$ is square integrable with respect to both variables $\mathbf{x}$ and $\mathbf{y}$ and is Y-periodic in the $\mathbf{y}$ variable (it belongs to $L^2\left(\Omega; \left(L^2_{\#}(Y)\right)^3\right)$). A complete analysis of this new mathematical tool can be found in [16].

We make the physically reasonable assumption that the electromagnetic energy remains bounded when η tends to 0, which is equivalent to assume that $(\mathbf{E}^\eta, \mathbf{H}^\eta)$ are both locally square integrable. Then it is known [16] that $(\mathbf{E}^\eta, \mathbf{H}^\eta)$ two-scale converges towards limit fields $(\mathbf{E}^0, \mathbf{H}^0)$. This physical assumption could be justified mathematically, however it seems quite obvious, from the point of view of physics, that the limit fields exist. The point is then to give the system of equations that is satisfied by these fields and to derive the effective permittivity and permeability tensors.

First of all, we have to determine the set of equations that are microscopically satisfied, that is, satisfied with respect to the hidden variable $\mathbf{y}$, for that will give the constitutive relations of the homogenized medium. Multiplying Maxwell-Faraday equation by a regular test function $\phi\left(\mathbf{x}, \frac{\mathbf{x}_\perp}{\eta}\right)$, and integrating over Ω, we obtain:

$$\int_\Omega \mathbf{E}^\eta(\mathbf{x}) . \left[\mathrm{curl}_x(\phi) + \frac{1}{\eta}\mathrm{curl}_y(\phi)\right] d\mathbf{x} = i\omega\mu_0 \int_\Omega \mu^\eta(\mathbf{x})\, \mathbf{H}^\eta(\mathbf{x})\, \phi(\mathbf{x}, \mathbf{x}_\perp/\eta)\, d\mathbf{x}. \tag{4}$$

Multiplying by η and letting η tend to 0, we get using (3):

$$\iint_{\Omega\times Y} \mathbf{E}^0(\mathbf{x}, \mathbf{y}) .\mathrm{curl}_y(\phi)\, d\mathbf{x}d\mathbf{y} = 0. \tag{5}$$

This is equivalent to:

$$\iint_{\Omega\times Y} \mathrm{curl}_y \mathbf{E}^0(\mathbf{x}, \mathbf{y}) .\phi(\mathbf{x}, \mathbf{y})\, d\mathbf{x}d\mathbf{y} = 0 \tag{6}$$

which is nothing else but the variational form for: $\mathrm{curl}_y \mathbf{E}^0 = 0$. In a very similar way, but using now Maxwell-Ampere equation, we get the equation: $\mathrm{curl}_y \mathbf{H}^0 = 0$. On the other hand, since $\varepsilon^\eta \mathbf{E}^\eta$ is divergence free, we have, for every test function $\phi(\mathbf{x}, \mathbf{y})$, $\int_\Omega \varepsilon^\eta(\mathbf{x})\, \mathbf{E}^\eta(\mathbf{x}) . \left[\nabla_x\phi + \frac{1}{\eta}\nabla_y\phi\right] d\mathbf{x} = 0$. Multiplying by η and letting η tend to 0, we get:

$$\iint_{\Omega\times Y} \varepsilon^\eta(\mathbf{y})\, \mathbf{E}^0(\mathbf{x}, \mathbf{y}) .\nabla_y\phi d\mathbf{x}d\mathbf{y} = 0, \tag{7}$$

this can be written as (notice that the div_y operator acts only on the transverse components):

$$\mathrm{div}_y\left(\varepsilon^0 \mathbf{E}^0\right) = 0. \tag{8}$$

Similarly, since the magnetic field is divergence free, we derive:

$$\mathrm{div}_y\left(\mu^0 \mathbf{H}^0\right) = 0. \tag{9}$$

Summing up, we have the following microscopic equations, holding inside the basic cell Y:

$$\begin{cases} \mathrm{div}_y\left(\mu^0 \mathbf{H}^0\right) = 0 \\ \mathrm{curl}_y \mathbf{H}^0 = 0 \end{cases}, \begin{cases} \mathrm{div}_y\left(\varepsilon^0 \mathbf{E}^0\right) = 0 \\ \mathrm{curl}_y \mathbf{E}^0 = 0 \end{cases} \tag{10}$$

The systems in (10) are respectively of electrostatic and magnetostatic types. This means that, with respect to the hidden variable $\mathbf{y}$, the electric field and magnetic field satisfy the static Maxwell system. This property is true only at that scale and not at the macroscopic scale. However, it is these static equations that determine the effective permittivity and permeability. Indeed let us analyze this system starting with the electric field. From the curl relation, we get $\nabla_y E_3^0 = 0$, and so $E_3^0(\mathbf{x}, \mathbf{y}) \equiv E_3(\mathbf{x})$. Besides, the basic cell having the geometry of a torus, we get the existence of a regular periodic function $w_E(\mathbf{y})$ such that:

$$\mathbf{E}_\perp^0 = \mathbf{E}_\perp + \nabla_y w_E. \tag{11}$$

The function w_E is the electrostatic potential associated with the microscopic electrostatic problem. Inserting (11) in equation (8) and projecting on the two horizontal axis, we obtain:

$$\mathrm{div}_y\left[\varepsilon^0\left(\mathbf{e}_i + \nabla_y w_{E,i}\right)\right] = 0,\ i \in \{1, 2\} \tag{12}$$

By linearity, denoting $\mathbf{E}_\perp = (E_1, E_2)$, we derive that the potential w_E is given by $w_E = E_1 w_{E,1} + E_2 w_{E,2}$, where $w_{E,i}$ are the periodic solutions of (12). Thus by (11):

$$\mathbf{E}^0(\mathbf{x}, \mathbf{y}) = \mathcal{E}(\mathbf{y})\, \mathbf{E}(\mathbf{x}) \tag{13}$$

where:

$$\mathcal{E}(\mathbf{y}) = \begin{pmatrix} 1 + \partial_{y_1} w_{E,1} & \partial_{y_1} w_{E,2} & 0 \\ \partial_{y_2} w_{E,1} & 1 + \partial_{y_2} w_{E,2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{14}$$

The magnetic field $\mathbf{H}^0$ can be handled in the same way since it satisfies exactly the same kind of equations as $\mathbf{H}^0$ (see (10)). In particular, we may represent its tranversal component in the form: $\mathbf{H}_\perp^0 = \mathbf{H}_\perp + \nabla_\perp w_H$, where w_H is a periodic magnetic potential (the possibility

of this representation is due to the curl-free condition which means that no microscopic current is present). Analogously as in (13,14), we find:

$$\mathbf{H}^0(\mathbf{x},\mathbf{y}) = \mathcal{M}(\mathbf{y})\,\mathbf{H}(\mathbf{x}) \tag{15}$$

with

$$\mathcal{M}(\mathbf{y}) = \begin{pmatrix} 1+\partial_{y_1}w_{H,1} & \partial_{y_1}w_{H,2} & 0 \\ \partial_{y_2}w_{H,1} & 1+\partial_{y_2}w_{H,2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{16}$$

where:

$$\mathrm{div}_y\left[\mu^0\left(\mathbf{e}_i + \nabla_y w_{H,i}\right)\right] = 0,\ i \in \{1,2\} \tag{17}$$

The above results show that, at the microscopic scale, the limit fields $(\mathbf{E^0},\mathbf{H^0})$ are completely determined by the physical fields $(\mathbf{E},\mathbf{H})$. Now that the microscopic behavior is precised, we are able to determine the macroscopic system satisfied by $(\mathbf{E},\mathbf{H})$. To that aim, let us choose a regular test function $\phi(x)$ independent of variable $\mathbf{y}$. From Maxwell equations we get

$$\begin{cases} \int_\Omega \mathbf{H}^\eta(\mathbf{x})\,.\mathrm{curl}(\phi)\,d\mathbf{x} = -i\omega\varepsilon_0\int_\Omega \varepsilon^\eta(\mathbf{x})\,\mathbf{E}^\eta(\mathbf{x})\,\phi(\mathbf{x})\,d\mathbf{x} \\ \int_\Omega \mathbf{E}^\eta(\mathbf{x})\,.\mathrm{curl}(\phi)\,d\mathbf{x} = i\omega\mu_0\int_\Omega \mu^\eta(\mathbf{x})\,\mathbf{H}^\eta(\mathbf{x})\,\phi(\mathbf{x})\,d\mathbf{x} \end{cases} \tag{18}$$

passing to the limit $\eta \to 0$, we get:

$$\begin{cases} \iint_{\Omega\times Y} \mathbf{H}^0(\mathbf{x},\mathbf{y})\,.\mathrm{curl}(\phi)\,d\mathbf{x}d\mathbf{y} = -i\omega\varepsilon_0\iint_{\Omega\times Y} \varepsilon^0(\mathbf{y})\,\mathbf{E}^0(\mathbf{x},\mathbf{y})\,\phi(\mathbf{x})\,d\mathbf{x}d\mathbf{y} \\ \iint_{\Omega\times Y} \mathbf{E}^0(\mathbf{x},\mathbf{y})\,.\mathrm{curl}(\phi)\,d\mathbf{x}d\mathbf{y} = i\omega\mu_0\iint_{\Omega\times Y} \mu^0(\mathbf{y})\,\mathbf{H}^0(\mathbf{x},\mathbf{y})\,\phi(\mathbf{x})\,d\mathbf{x}d\mathbf{y} \end{cases} \tag{19}$$

Recalling that $\langle\mathbf{E}^0\rangle = \mathbf{E}$ and that $\langle\mathbf{H}^0\rangle = \mathbf{H}$, we get:

$$\begin{cases} \mathrm{curl}\ \mathbf{E} = i\omega\mu_0\langle\mu^0\mathbf{H}^0\rangle \\ \mathrm{curl}\ \mathbf{H} = -i\omega\varepsilon_0\langle\varepsilon^0\mathbf{E}^0\rangle \end{cases} \tag{20}$$

which, taking into account (13,15), brings to the limit system:

$$\begin{cases} \mathrm{curl}\ \mathbf{E} = i\omega\mu_0\langle\mu^0\mathcal{M}\rangle\,\mathbf{H} \\ \mathrm{curl}\ \mathbf{H} = -i\omega\varepsilon_0\langle\varepsilon^0\mathcal{E}\rangle\,\mathbf{E} \end{cases} \tag{21}$$

The homogenized permeability and permittivity tensors are thus respectively $\langle\mu^0\mathcal{M}\rangle$ and $\langle\varepsilon^0\mathcal{E}\rangle$. It appears here that the homogenization process is purely local, and that the finiteness

of the fibers does not play any role in the homogeneous properties of the medium: the effective tensors coincide with that obtained in the polarized cases [3, 10, 17]. This surprising property is easily foreseen by our methodology. An approach relying on explicit calculations, for instance using Bloch-waves theory or Fourier-Bessel expansions, cannot work here, due the lack of an explicit representation of the fields in case of finite size fibers. It should also be noted that the case of materials with losses is handled by our result. This result can be straightforwardly applied to the study of membrane photonic crystal in the long wavelength range where phenomena of birefringence and dichroism are obtained [18]. However, we emphasize that the locality pointed out, that is, the fact the effective constitutive relations are local ones, is lost if we change the scale of the permittivity coefficients in the obstacles. In particular, the results obtained in the case of infinite conductivities in the polarized case [10] cannot be transposed to the case of fibers with finite length, due to the emergence of surprising non local effects which are studied in [21, 22]. We also remark that the situation that we handle here is different from that studied in [20] where the small parameter is the depth over wavelength, while the period over wavelength ratio is not small, contrarily to our situation. In that case, a dependence on the depth is found. In our homogenization result, it is clear that the main numerical problem is the solving of the annex problems (12,17) for they give the effective matrices $\mathcal{E}$ and $\mathcal{M}$. In certain simple cases, for instance that of circular isotropic non magnetic rods and a permittivity constant in each connected region, it is possible to find an explicit expression for the effective permittivity (it is in fact a very old problem). However, for more complicated geometries, there is a general numerical procedure based on fictitious sources, that allows to solve both annex problems at a low numerical cost [23].

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Figures captions

Figure 1: Schematics of the photonic crystal

Figure 2: Schematics of the basic cells.

(a) Tridimensional basic cell with cylindrical obstacle.

(b) Bidimensional basic cell Y with 2D obstacle P.

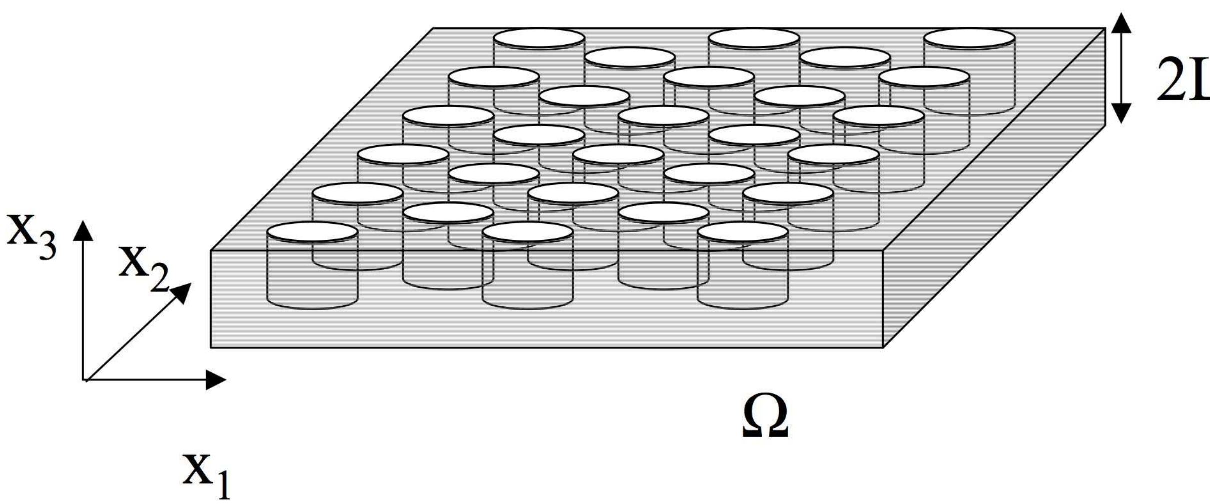

Figure 1

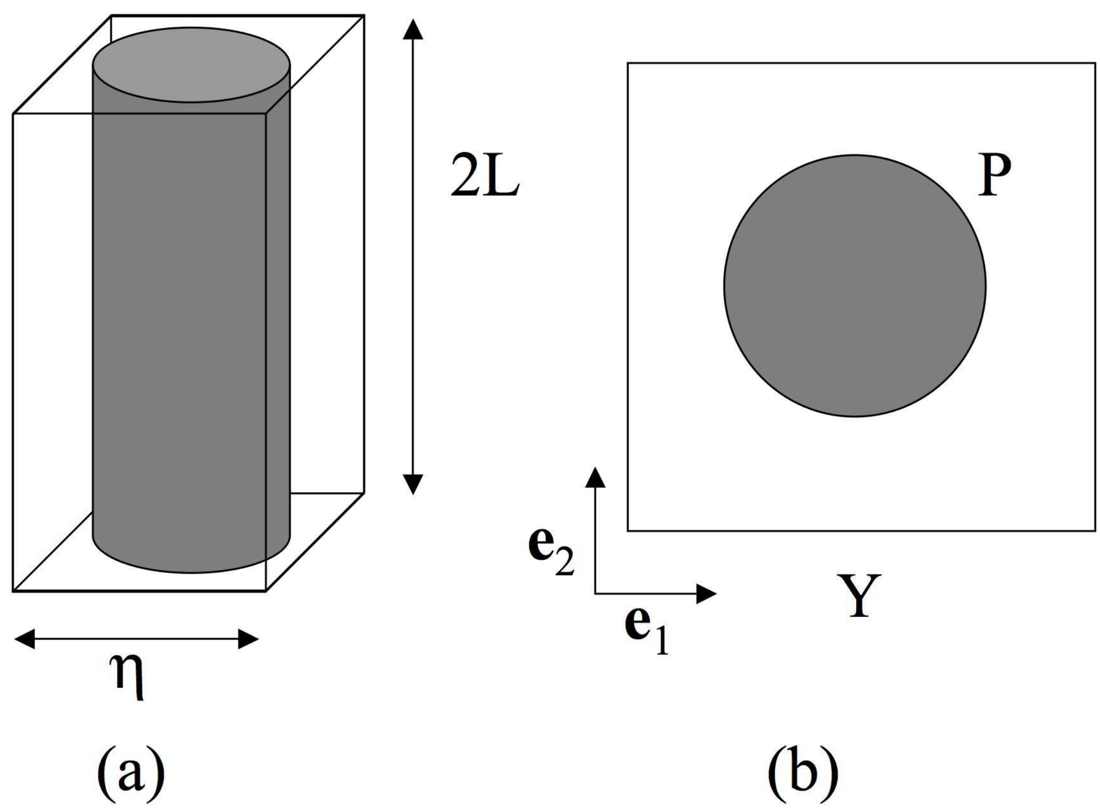

Figure 2